Effects of constraints on the phase transition to Bose-Einstein condensation

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Abstract

Classic and recent results for the critical behaviour of ideal Bose gas at constant volume and constant pressure and for various spatial dimensionalities $d > 0$ are reviewed. New results about the critical properties in a close vicinity of the $\lambda-$point are presented.

PACS: 03.75Hh, 05.70.Ce, 05.70.Jk
Key words: free energy, equation of state, susceptibility

1 Introduction

The thermodynamic potential and the correlation functions of ideal Bose gas (IBG) [1, 2] were studied in a number of preceding papers [3, 4, 5, 6, 7, 8, 9, 10]; see also the review [11]. In this paper we shall present a brief review of known results together with an unified treatment of critical properties of IBG based on the derivation of effective free energy of Landau-Ginzburg type. Our consideration makes possible to outline a general picture of the critical behaviour of IBG as well as to present some new results about the effects of thermodynamic constraints: the conditions of constant volume ($V = const$) and constant pressure ($P = const$) for certain spatial dimensionalities ($d > 0$). We should emphasize that the thermodynamic behaviour of IBG near the $\lambda-$point corresponds either to a phase transition of first order or, in cases which we shall enumerate, resembles a continuous phase transition that is not equivalent to the standard second order phase transition described by φ^4-model (see, e.g., Ref. [2]). Our results could be used in the interpretation of thermodynamic behaviour of extremely dilute Bose-Einstein condensates (BEC), where the interparticle interaction can be neglected.

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2 Thermodynamic potential

We consider noninteracting and homogeneous gas of spinless bosons, described by the Hamiltonian [3, 4, 6]

$$\hat{H} = \sum_{\vec{k}} \left[(\epsilon_k + r)\hat{a}_{\vec{k}}^+ \hat{a}_{\vec{k}} - \frac{1}{\sqrt{N}} (\hat{a}_0^+ h + \hat{a}_0 h^*) \right], \tag{1}$$

where $r = -\mu \geq 0$ is the modulus of the chemical potential μ, $\vec{k} = \{k_j; j = 1, ..., d\}$ is the d-dimensional wave vector, $\hat{a}_{\vec{k}}$ and $\hat{a}_{\vec{k}}^+$ are second quantization operators, and N is the total number of bosons. The external field h generates the spontaneous symmetry breaking ($\langle \hat{a}_0 \rangle > 0$) below the critical temperature T_c. The energy spectrum $\epsilon_k = ck^\sigma$ includes two cases: (i) $\sigma = 2$, corresponding to real boson particles and boson excitations produced by short-range interparticle (fermion and spin) interactions, and (ii) $0 < \sigma < 2$, which stands for boson excitations (composite bosons) produced by long-range interparticle interactions (see, e.g., Refs. [2, 11]). The parameter c is equal to $(\hbar^2/2m)$, where m is the effective mass of the bosons.

The grand canonical thermodynamic potential of IBG,

$$\Omega(T, r, h) = -\beta^{-1} \ln \text{Tr} \exp\left(-\beta \hat{H}\right), \tag{2}$$

can be exactly calculated [3, 4, 6]. This quantity can be written in general form

$$\Omega(T, r, h) = -\beta^{-1} V \lambda_T^{-d} A(d, \sigma) g_{d/\sigma+1}(\beta r) - \frac{1}{N} \frac{hh^*}{r}, \tag{3}$$

where $\lambda_T = (2\pi\hbar^2/mk_B T)^{1/\sigma}$ is the thermal wavelength,

$$g_\nu(y) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1}}{e^{x+y} - 1} dx \tag{4}$$

is the integral Bose function (see, e.g., [2]) and

$$A(d, \sigma) = \frac{2^{1-d+2d/\sigma} \Gamma(d/\sigma)}{\sigma \pi^{d(1/2-1/\sigma)} \Gamma(d/2)} \tag{5}$$

is a constant with the property $A(d, 2) = 1$. Note, that the grand potential (3) obeys differential relation $d\Omega(T, r, h) = -SdT + Ndr - \Psi dh^* - \Psi^* dh$, where S is the entropy and ($\Psi \sim \langle \hat{a}_0 \rangle$) is the order parameter of BEC.

The free energy $\widetilde{\Omega}(T, r, \Psi)$, in which the natural thermodynamic variable is the order parameter Ψ, can be obtained from $\Omega(T, r, h)$ through the standard Legendre transformation

$$\widetilde{\Omega}(T, r, \Psi) = \Omega(T, r, h) + h\Psi^* + h^*\Psi|_{h(\Psi)}, \tag{6}$$

where

$$\Psi = -\frac{\partial \Omega}{\partial h^*} = \frac{h}{Nr}, \quad \Psi^* = -\frac{\partial \Omega}{\partial h} = \frac{h^*}{Nr}. \tag{7}$$

Using Eqs. (3)-(7) we obtain

$$\widetilde{\Omega}(T, r, \Psi) = -\beta^{-1}V\lambda_T^{-d}A(d, \sigma)g_{d/\sigma+1}(\beta r) + Nr\Psi^2. \tag{8}$$

We can restrict our calculations without a loss of generality to real values of h and Ψ. The susceptibility is given by $\chi_T = \partial\Psi/\partial h = 1/Nr \sim t^{-\gamma}$, where γ is the susceptibility critical exponent and $t = (T - T_c)/T_c$ (see, e.g., [2]).

For small r and energies ($\epsilon_k \ll k_B T$) the correlation function $\chi(k) = \beta N^{-1}\langle \hat{a}_{\vec{k}}^+ \hat{a}_{\vec{k}} \rangle$ takes the form $N^{-1}(ck^\sigma + r)^{-1}$. This gives the correlation length $\xi = (c/r)^{1/\sigma} \sim t^{-\nu}$ and $\chi(k) \sim k^{-\sigma}$ at $r = 0$. From $\chi(k) \sim k^{-\sigma}$ we obtain that the Fisher exponent η, defined by $\chi(k) \sim k^{-2+\eta}$, is equal to $(2-\sigma)$ for all dimensional ranges and constraints (see Table 1). In order to obtain the correlation length exponent ν and the exponent γ of susceptibility χ_T, we need to derive the function $r(t)$ for a general spatial dimensionality d for cases of constant volume and constant pressure. The nullifying of chemical potential defines the critical temperature T_c of BEC for both cases ($V = const$, $P = const$).

3 Constant volume

For the thermodynamic condition of constant volume we need the free energy $f(T, N/V, \Psi)$, in which the natural variable is the volume V (or the number density N/V). To obtain it we expand the integral Bose function $g_\nu(y)$ in powers of βr and express the chemical potential as a function of the volume (or density). We expand the function g_ν in the potential $\widetilde{\Omega}$ to the same order in βr. This allows to make the next Legendre transformation

$$f(T, N/V, \Psi) = \widetilde{\omega}(T, r, \Psi) - \frac{N}{V}r|_{r(N/V)}, \tag{9}$$

where

$$\frac{N}{V} = \frac{\partial\widetilde{\omega}}{\partial r} = \lambda_T^{-d}A(d, \sigma)g_{d/\sigma}(\beta r) + \frac{N}{V}\Psi^2, \tag{10}$$
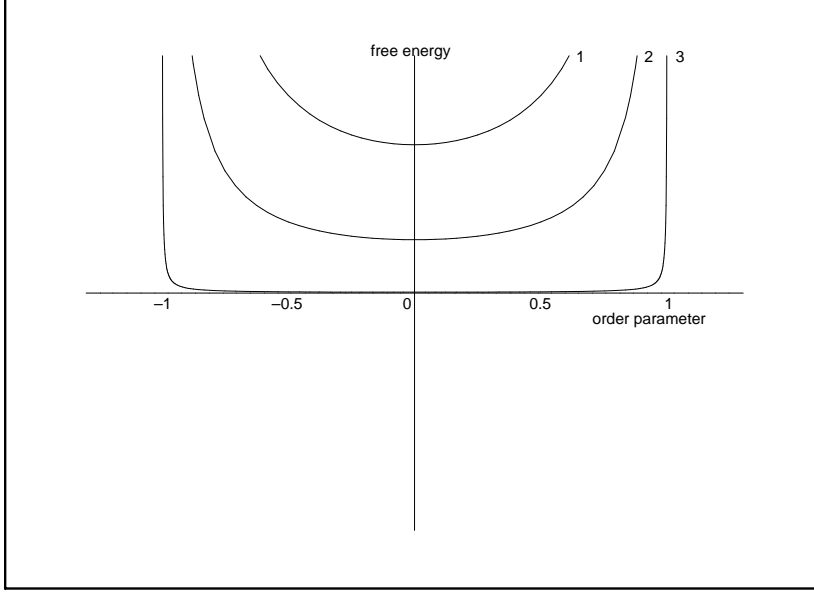
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Figure 1: Effective free energy for $d < \sigma$ $(d = 1, \sigma = 2)$, $V = const$: line 1 $(T = 0.25)$, line 2 $(T = 0.15)$, line 3 $(T = 0.02)$. The case $d = \sigma$ is qualitatively the same.

$f = F/V$ and $\widetilde{\omega} = \widetilde{\Omega}/V$. Subtracting the free energy of the disordered phase f_{dis} we obtain the following effective free energies corresponding to several dimensionality ranges:

$$
\begin{aligned}
f(T, N/V, \Psi) &\sim \frac{T^{\sigma/(\sigma-d)}}{(1 - \Psi^2)^{d/(\sigma-d)}} & d &< \sigma \\
&\sim T^2\exp\left(-\frac{1 - \Psi^2}{T}\frac{N}{\lambda_0^{-d}A(d,\sigma)V}\right) & d &= \sigma \\
&\sim -\left(-\Psi^2 - \frac{d}{\sigma}t\right)^{d/(d-\sigma)} & \sigma &< d < 2\sigma \\
&\sim (\Psi^2 + 2t)^2\frac{1}{\ln(\Psi^2 + 2t)^{-1}} & d &= 2\sigma \\
&\sim \left(\frac{\sigma}{d}\Psi^2 + t\right)^2 & d &> 2\sigma.
\end{aligned}
\tag{11}
$$

The case $d < \sigma$ is depicted in Fig. 1 for $d = 1$ and $\sigma = 2$. We take the volume per particle $v = V/N$ to be unity and $m = \hbar = k_B = 1$. The number coefficient in Eq. (11) is equal to $1/2$ and $T_c = 0$. When the temperature tends to zero the curve $f(\Psi)$ acquires a flat part, indicating that the order parameter Ψ occurs with a jump at $T_c = 0$. In Fig. 2 we show the $d > 2\sigma$ case, when $d = 5$ and $\sigma = 2$. Now the numerical factor in Eq. (11) is 8.96 and the normalization $\widetilde{\Psi} = \sqrt{\sigma/d}\Psi$ has been used. The function $f(\Psi)$, shown in Figs. 1 and 2, is quite different from the respective potential $f(\Psi)$ known for the usual cases of IBG $(d = 3, \sigma = 2)$ [4] and the φ^4-model [2].

Using the free energy (11) we calculate the specific heat at constant volume $C_V = -T(\partial^2 f/\partial T^2)$ and the equation of state $h = \partial f/\partial\Psi$. Bearing in mind the definitions
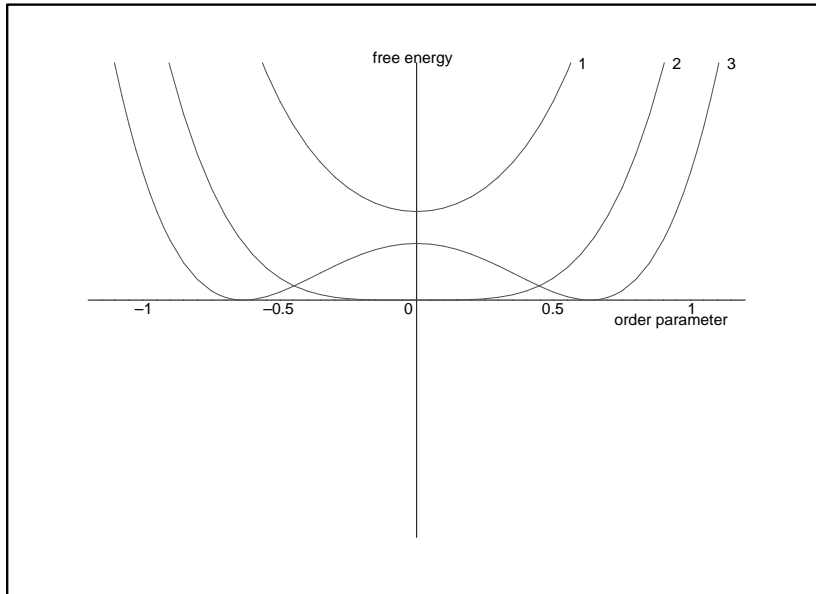
Figure 2: Effective free energy for $d > 2\sigma$ $(d = 5, \sigma = 2)$, $V = const$: line 1 $(t = 0.5)$, line 2 $(t = 0)$, line 3 $(t = -0.4)$. The case $d = 2\sigma$ is qualitatively the same.

(see, e.g., [2]), $C_V \sim t^{-\alpha}$, $\Psi \sim h^{1/\delta}$ $(h \sim 0)$ and $\Psi \sim t^{\beta}$ $(h = 0)$ we obtain the critical exponents α, δ and β. The values of the critical exponents are given in Table 1[1]. The behaviour of Ψ, V, S, C_V and χ_T at T_c is given in Table 2.

4   Constant pressure

When the system is under constant pressure we should use the free energy per particle μ, in which the natural variable is the pressure P . To obtain the chemical potential we solve the equation for the pressure $P = -\partial \widetilde{f}/\partial v$ with respect to the volume per particle v to the lowest order in t. Thus we make the following Legendre transformation

$$\mu(T, P, \Psi) = \widetilde{f}(T, N/V, \Psi) + Pv|_{v(P)}, \tag{12}$$

where $\mu = \Phi/N$ and $\widetilde{f} = F/N = fv$.

For the various dimensional ranges we obtain

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[1]In Table 1 we distinguish logarithmic factors by "exponents" with suffix l. Thus $f(t)$ is said to have exponent x_l or x^l, respectively, if $f(t) \sim t^x/\ln t^{-1}$ or $f(t) \sim t^x \ln t^{-1}$ [3].
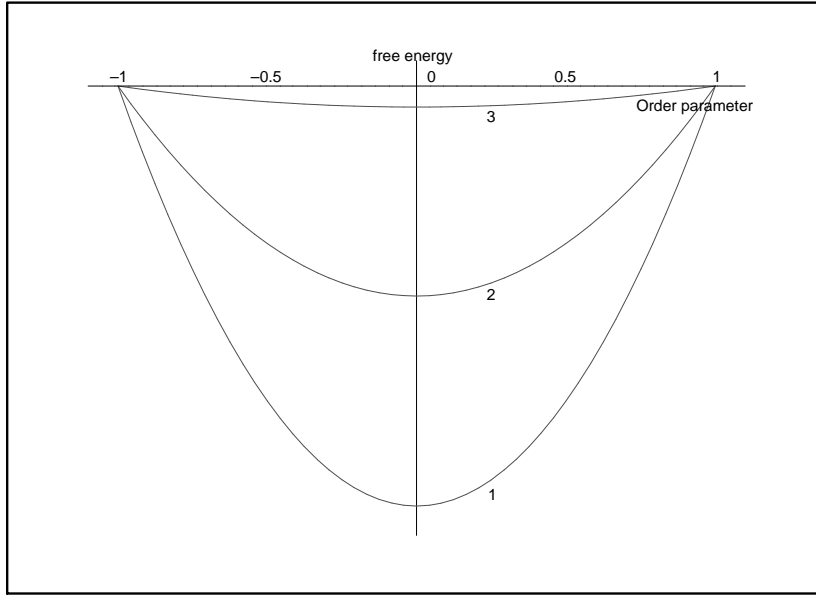
Figure 3: Effective thermodynamic potential for $d > \sigma$ $(d = 3, \sigma = 2)$, P=const: line 1 $(t = 0.1)$, line 2 $(t = 0.05)$, line 3 $(t = 0.005)$. The case $d \leq \sigma$ is qualitatively the same.

$$
\begin{aligned}
\mu(T, P, \Psi) &\sim -(1 - \Psi^2)t^{\sigma/d}(1 + at) & d &< \sigma \\
&\sim -(1 - \Psi^2)\frac{t + at^2}{\ln t^{-1}} & d &= \sigma \\
&\sim -(1 - \Psi^2)t(1 + at^{d/\sigma - 1}) & \sigma &< d < 2\sigma \\
&\sim -(1 - \Psi^2)t + (1 - \Psi^2)t^2(1 + at)\ln t^{-1} & d &= 2\sigma \\
&\sim -(1 - \Psi^2)t - (1 - \Psi^2)t^2(1 + at^{d/\sigma - 2} + bt) & d &> 2\sigma.
\end{aligned}
\tag{13}
$$

In Fig. 3 we depict the case $\sigma < d < 2\sigma$ for $d = 3$ and $\sigma = 2$. We set again $m = \hbar = k_B = 1$ and take the magnitude of the pressure P so as to give $T_c = 1$. This gives the factor 1.28 for the coefficient of proportionality in Eq. (13). This picture should be compared with those shown in Figs. 1 and 2 (see, also, [2, 4]).

We derive from the free energy μ the specific heat at constant pressure $C_P = -T(\partial^2 \mu / \partial T^2)$ and the exponent α. Moreover the chemical potential (13) can be used to calculate the correlation length and susceptibility exponents ν and γ. Since the order parameter has a jump, as is seen from Eq. (13) (μ is zero below T_c), the exponents β and δ cannot be defined. The values of the critical exponents and the behaviour of Ψ, V, S, C_P and χ_T at T_c are given in Tables 1 and 2.

6

5 Summary

In this paper we derived and analyzed the IBG free energies of Landau-Ginzburg type for the thermodynamic constraints of constant volume and constant pressure at different spatial dimensionalities $d > 0$. The values of the critical exponents for various spatial dimensionalities are given in Table 1. The critical exponents for $d = (\sigma, 2\sigma)$ and $P = const$ are new results of our investigation. The derived free energies enable us to present the behaviour of thermodynamic functions at the critical point. It is shown in Table 2. Besides, our results make possible to estimate the order of the phase transition to BEC. When $d > \sigma$ and $P = const$ this phase transition is of first order. But for lower dimensionalities ($d \leq \sigma$) and in both cases ($P = const, V = const$), the phase transition to BEC resembles a first order phase transition only by the order parameter jump. On the other hand, for $d > \sigma$ and $V = const$ the phase transition to BEC is a continuous phase transition with properties, which are quite different from the properties of the standard second order phase transition described by φ^4-model. Our results can be used in the interpretation of experimental results for BEC in extremely dilute boson gases at constant pressure or volume.

TABLE 1. Critical exponents of the ideal Bose gas.

VOLUME=const	α	α_s	β	γ	δ	ν	η
$d < \sigma$ $(T_c = 0)$	$-d/\sigma$	$-$	$*$	$\frac{\sigma}{\sigma-d}$	$*$	$\frac{1}{\sigma-d}$	$2 - \sigma$
$d = \sigma$ $(T_c = 0)$	-1	$-$	$*$	∞	$*$	∞	$2 - \sigma$
$\sigma < d < 2\sigma$ $(T_c > 0)$	0	$\frac{d-2\sigma}{d-\sigma}$	$1/2$	$\frac{\sigma}{d-\sigma}$	$\frac{d+\sigma}{d-\sigma}$	$\frac{1}{d-\sigma}$	$2 - \sigma$
$d = 2\sigma$ $(T_c > 0)$	0	0_l	$1/2$	1_l	3_l	$\sigma\nu = 1_l$	$2 - \sigma$
$d > 2\sigma$ $(T_c > 0)$	0	$(\frac{2\sigma-d}{\sigma}, -1)^a$	$1/2$	1	3	$1/\sigma$	$2 - \sigma$
PRESSURE=const	α	α_s	β	γ	δ	ν	η
$d < \sigma$ $(T_c > 0)$	$2 - \sigma/d$	-1^b	$*$	σ/d	$*$	$1/d$	$2 - \sigma$
$d = \sigma$ $(T_c > 0)$	0_l	$-$	$*$	1_l	$*$	$\sigma\nu = 1_l$	$2 - \sigma$
$\sigma < d < 2\sigma$ $(T_c > 0)$	$2 - d/\sigma$	$-$	$*$	1	$*$	$1/\sigma$	$2 - \sigma$
$d = 2\sigma$ $(T_c > 0)$	0	0^l	$*$	1	$*$	$1/\sigma$	$2 - \sigma$
$d > 2\sigma$ $(T_c > 0)$	0	$(\frac{2\sigma-d}{\sigma}, -1)^a$	$*$	1	$*$	$1/\sigma$	$2 - \sigma$

*The order parameter has a jump (from 0 to 1) at T_c.
[a]The first entry is for $d < 3\sigma$, the second is for $d > 3\sigma$.
[b]This entry is only for $d = \sigma/2$.

TABLE 2. Behaviour of Ψ, V, S, C_V, C_P, χ_T at T_c.

VOLUME=const	order par.	volume	entropy	heat cap.	suscept.
$d < \sigma$ $(T_c = 0)$	jump	const.	cont.	cont.	diverg.
$d = \sigma$ $(T_c = 0)$	jump	const.	cont.	cont.	diverg.
$\sigma < d < 2\sigma$ $(T_c > 0)$	cont.	const.	cusp	cusp	diverg.
$d = 2\sigma$ $(T_c > 0)$	cont.	const.	cusp	cusp	diverg.
$d > 2\sigma$ $(T_c > 0)$	cont.	const.	cusp	cusp	diverg.
PRESSURE=const	order par.	volume	entropy	heat cap.	suscept.
$d < \sigma$ $(T_c > 0)$	jump	cont.	cont.	cont/jump/div.[a]	diverg.
$d = \sigma$ $(T_c > 0)$	jump	cont.	cont.	cont.	diverg.
$\sigma < d < 2\sigma$ $(T_c > 0)$	jump	jump	jump	divergent	diverg.
$d = 2\sigma$ $(T_c > 0)$	jump	jump	jump	ln divergent	diverg.
$d > 2\sigma$ $(T_c > 0)$	jump	jump	jump	jump	diverg.

[a]Respectively for $d < \sigma/2$, $d = \sigma/2$, $d > \sigma/2$.

Acknowledgments

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